NsG-512

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For the period October 1, 1963-March 31, 1964; NASA Research Grant NsG-512 to the University of Florida for basic scientific research on the subject:

"Quantum Theory Studies of the Energies of Excited State Atoms and Molecules, Particularly as They Occur in the Upper and Stellar Atmospheres, and in Materials Undergoing Combustion."

During the first six-month period, the essential point was to get the contracted research started. Due to previous planning, sufficient scientific personnel was available almost from the very beginning or could be brought to the University of Florida during the fall. The main emphasis has been on the study of the fundamental quantum theory of excited states of simple atoms and molecules as are present in the upper atmosphere, and particularly on the theory for excited states. Special attention has been paid to the problem of finding both upper and lower bounds for the energy values of the stationary states, as well as for other quantities. A great deal of effort has been devoted to the study of the so-called "partitioning technique" which is the stronger equivalent to infinite-order perturbation theory. This approach was outlined in the research proposal, and it has been possible for us to make considerable extensions and generalizations. In addition, fundamental problems connected with the time-dependent Schrödinger equation have been studied, particularly elementary atomic and molecular collisions and their relations to chemical kinetics. After this summary, the various aspects of the research carried out will be sketched in somewhat greater detail.

The project was fortunate in getting Professor Kimio Ohno of the University of Tokyo as Associate Director and first co-investigator on this grant. Professor Ohno comes from Professor Kotani's group, and

he has also studied and carried out research two years in England and two years in Sweden. He is a very fine expert on self-consistent-field calculations for atoms, small molecules, and conjugated systems. Professor Ohno arrived in Florida around November 15, 1963, and he took as his first duty to get in contact with the other research groups in the United States working on self-consistent-field problems. He studied the work on the evaluation of atomic and molecular integrals by means of electronic computers, and saw that the programs available would be adapted to the IBM 709 machine in Gainesville.

Professor Joseph O. Hirschfelder of the University of Wisconsin joined the project for two months as Visiting Research Professor. During his stay in Florida, the group thoroughly discussed the modern aspects on perturbation theory--both lower-order perturbation theory of the Lewis-Dalgarno type, and infinite-order perturbation theory. Professor Hirschfelder lectured also about fundamental chemical kinetics from the point of view of quantum theory. Professor Hirschfelder's visit was most valuable to our research efforts.

The problems of molecular collisions in the upper atmosphere has also been attacked by Dr. Ludwig Hofacker and Professor Akiko Ohno. Dr. Hofacker was particularly interested in the definition of the concept of potential energy surfaces and reaction paths, and Mrs. Ohno has studied the pressure broadening of spectral lines due to such collisions. Both studies have been successful and will in due time be reported in publications.

In the treatment of stationary states, the variation principle usually provides good upper bounds for the energy values. For many decades it has been a fundamental but very difficult problem to find

also lower bounds to these energy values. In the research proposal, I pointed out the importance of the so-called "bracketing theorem" giving upper and lower bounds to the energy values, but it seemed very difficult to apply this method in practice, depending on the fact that one would have to deal with infinite-order matrices. This problem has been solved during the month of March by combining the partitioning technique with the Weinstein method of intermediate Hamiltonians. Weinstein and his associates, Aronozajn, Fox, and Bazley, have during the last decade made important progress in the theory of lower bounds and, by combining their projection technique with the partitioning formula for the energy, I have been able to derive an explicit expression for successive approximations to energy levels from below. The technique has been applied to the electronic computer by Dr. Jack G. Gay and has proven to be quite successful. It is my intention to write a technical report about this research within the nearest future.

Dr. J. G. Gay worked on the problem of lower bounds for his Ph.D. thesis, which he finished in December 1963. He has also prepared a manuscript for publication with the title, "A Lower Bound Procedure for Energy Eigenvalues" and this work will be partially credited to the NASA grant. Reprints will be submitted as soon as they are available.

As technical and editorial assistant, the project has acquired Mrs. Eleanor J. Fox who is a most valuable helper in our research efforts.

During the next six months we plan to continue the research along the same lines, and we sincerely hope for an extension of the contract

on October 1, 1964 in accordance with the original plans.

The two Ohnos will leave the project on August 31, 1964, to return to Japan to assume professorships at the University of Hokkaido in Sapporo. As Associate Director the group has been successful in acquiring Professor Ruben Pauncz of the Technion-Haifa, Israel, who will spend two years with the Florida Project starting September 1, 1964.

The Quantum Theory Project at the University of Florida is undergoing another important extension on September 1, 1964 since Professor John C. Slater of M.I.T. is going to join the project for eight months a year, spending four months at M.I.T. Even if he will not be directly associated with the research on the NASA grant, I am sure that his presence will be highly beneficial for the research supported under this grant in the form of discussions and ideas.

A fiscal report will be sent directly from the University Business Office.

3/31/64 Per-Olov Löwdin